



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 4, 2024 – 06:25 pm BST

PDB ID : 6HD6  
Title : ABL1 IN COMPLEX WITH COMPOUND6 AND IMATINIB (STI-571)  
Authors : Cowan-Jacob, S.W.  
Deposited on : 2018-08-17  
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : **FAILED**  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

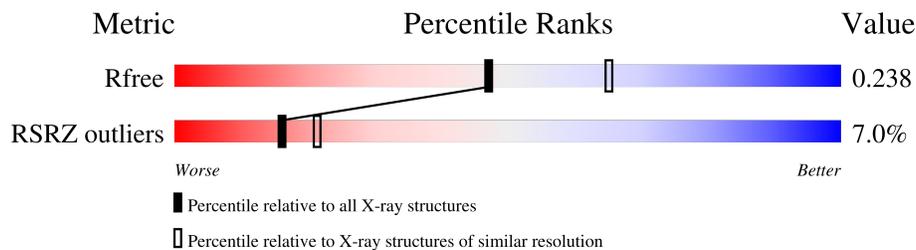
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5042 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5135 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tyrosine-protein kinase ABL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	285	2322	1492	375	437	18	0	2	0
1	B	283	2299	1478	372	431	18	0	0	0

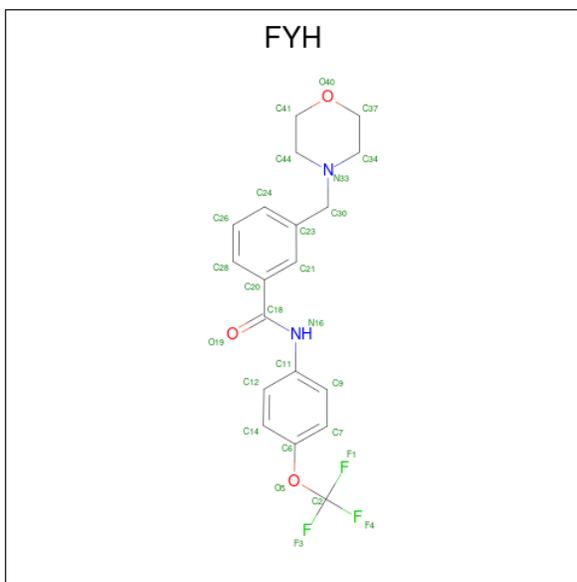
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	242	GLY	-	expression tag	UNP P00520
A	243	ALA	-	expression tag	UNP P00520
A	244	MET	-	expression tag	UNP P00520
A	245	ASP	-	expression tag	UNP P00520
A	246	PRO	-	expression tag	UNP P00520
A	247	SER	-	expression tag	UNP P00520
B	242	GLY	-	expression tag	UNP P00520
B	243	ALA	-	expression tag	UNP P00520
B	244	MET	-	expression tag	UNP P00520
B	245	ASP	-	expression tag	UNP P00520
B	246	PRO	-	expression tag	UNP P00520
B	247	SER	-	expression tag	UNP P00520

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

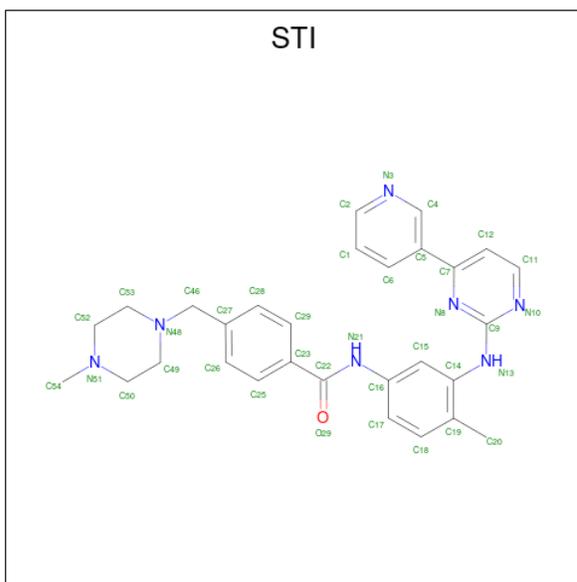
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is 3-(morpholin-4-ylmethyl)- {N}-[4-(trifluoromethoxy)phenyl]benzamide (three-letter code: FYH) (formula: C<sub>19</sub>H<sub>19</sub>F<sub>3</sub>N<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	F	N			O
3	A	1	54	38	6	4	6	0	1

- Molecule 4 is 4-(4-METHYL-PIPERAZIN-1-YLMETHYL)-N-[4-METHYL-3-(4-PYRIDIN-3-YL-PYRIMIDIN-2-YLAMINO)-PHENYL]-BENZAMIDE (three-letter code: STI) (formula: C<sub>29</sub>H<sub>31</sub>N<sub>7</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	37	29	7	1	0	0
4	B	1	37	29	7	1	0	0

- Molecule 5 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	A	258	Total 258	O 258	0	0
5	B	127	Total 127	O 127	0	0

MolProbity failed to run properly - this section is therefore empty.

### 3 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.08Å 65.20Å 66.35Å 73.30° 79.82° 84.54°	Depositor
Resolution (Å)	35.25 – 2.30 33.75 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.6 (35.25-2.30) 94.6 (33.75-2.30)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.13 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.3.0040	Depositor
R, $R_{free}$	0.175 , 0.238 0.174 , 0.238	Depositor DCC
$R_{free}$ test set	1397 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.9	Xtrriage
Anisotropy	0.153	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 62.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5135	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.83% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 4.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FYH	A	602[B]	-	29,29,29	1.00	1 (3%)	40,40,40	1.09	3 (7%)
4	STI	B	601	-	40,41,41	0.98	2 (5%)	51,56,56	2.12	10 (19%)
3	FYH	A	602[A]	-	29,29,29	1.12	2 (6%)	40,40,40	1.23	5 (12%)
4	STI	A	603	-	40,41,41	1.12	2 (5%)	51,56,56	2.01	10 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FYH	A	602[B]	-	-	6/17/25/25	0/3/3/3
4	STI	B	601	-	-	1/16/30/30	0/5/5/5
3	FYH	A	602[A]	-	-	2/17/25/25	0/3/3/3
4	STI	A	603	-	-	2/16/30/30	0/5/5/5

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	STI	C7-N8	-2.40	1.33	1.37
3	A	602[A]	FYH	O5-C2	2.30	1.44	1.31
3	A	602[B]	FYH	O5-C2	2.29	1.44	1.31
3	A	602[A]	FYH	C30-C23	2.25	1.55	1.51
4	B	601	STI	C46-C27	2.09	1.55	1.51

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	STI	N10-C9-N8	-7.59	119.19	126.52
4	B	601	STI	C11-N10-C9	7.24	121.87	115.45
4	A	603	STI	C11-N10-C9	6.86	121.54	115.45
4	A	603	STI	N10-C9-N8	-6.81	119.94	126.52
4	A	603	STI	C12-C11-N10	-5.21	118.67	123.81

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603	STI	C15-C14-N13-C9
3	A	602[A]	FYH	C23-C30-N33-C44
3	A	602[A]	FYH	C23-C30-N33-C34
3	A	602[B]	FYH	C23-C30-N33-C44
3	A	602[B]	FYH	N16-C18-C20-C28

There are no ring outliers.

No monomer is involved in short contacts.

#### 4.7 Other polymers [i](#)

There are no such residues in this entry.

#### 4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 5 Fit of model and data [i](#)

### 5.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	285/293 (97%)	-0.06	5 (1%) 68 74	10, 24, 49, 68	0
1	B	283/293 (96%)	0.52	35 (12%) 4 5	20, 41, 69, 80	0
All	All	568/586 (96%)	0.22	40 (7%) 16 21	10, 33, 66, 80	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	297	MET	7.2
1	B	407	MET	7.1
1	B	416	ALA	5.9
1	B	414	ALA	5.8
1	B	408	THR	4.5

### 5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.3 Carbohydrates [i](#)

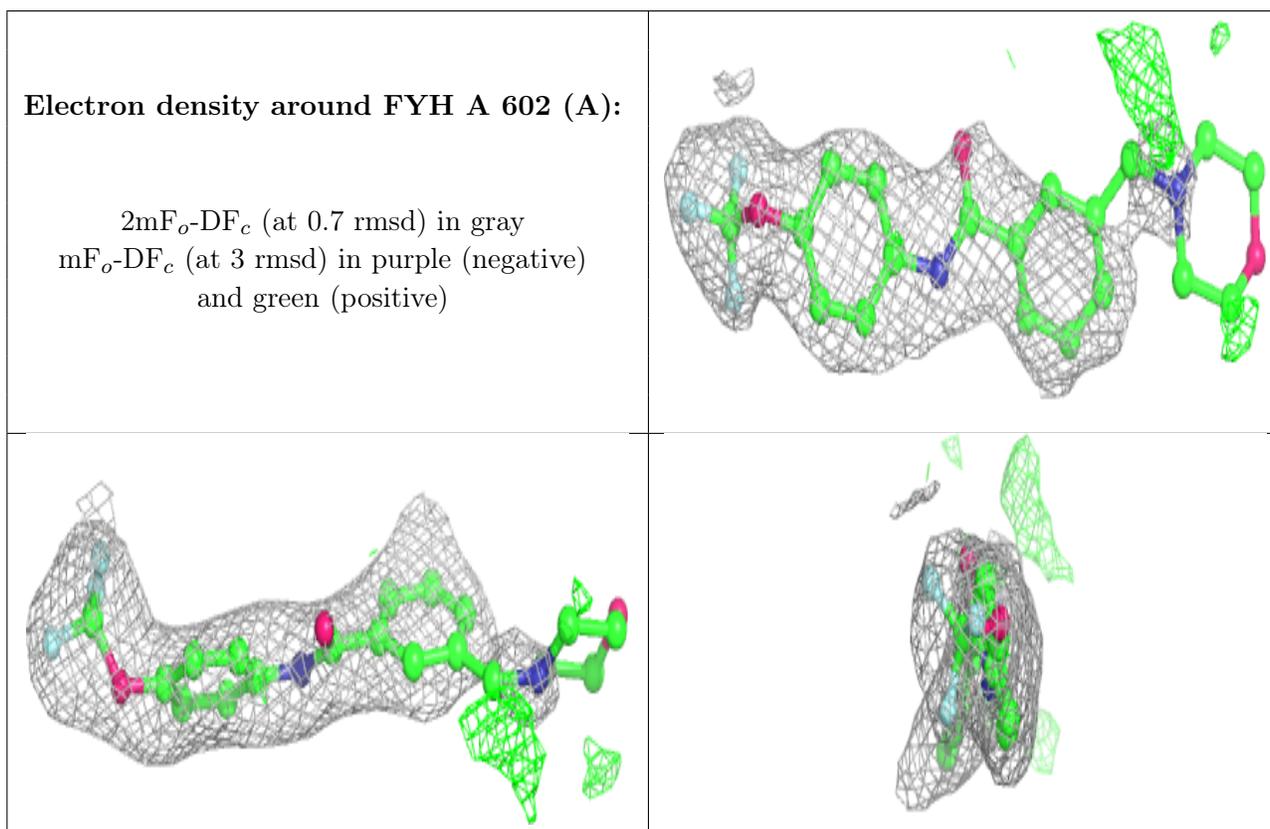
There are no monosaccharides in this entry.

### 5.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

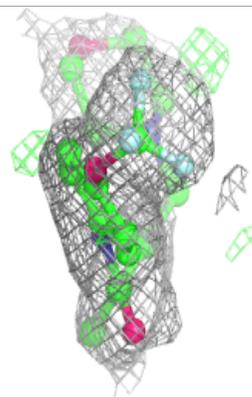
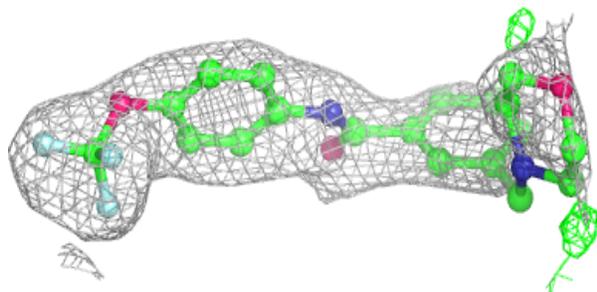
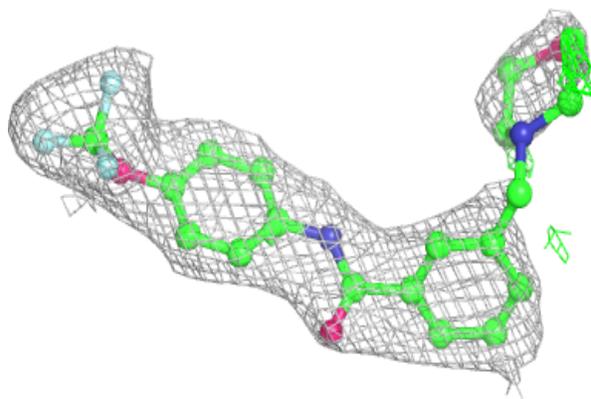
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FYH	A	602[A]	27/27	0.94	0.29	32,40,51,52	27
3	FYH	A	602[B]	27/27	0.94	0.29	23,28,30,31	27
4	STI	A	603	37/37	0.96	0.14	13,16,20,20	0
4	STI	B	601	37/37	0.96	0.12	24,30,37,37	0
2	CL	A	601	1/1	0.99	0.07	30,30,30,30	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

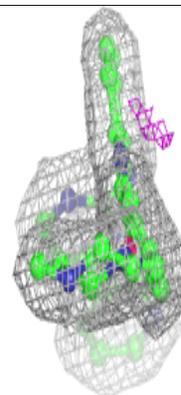
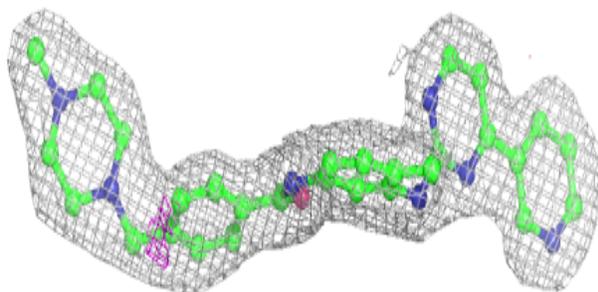
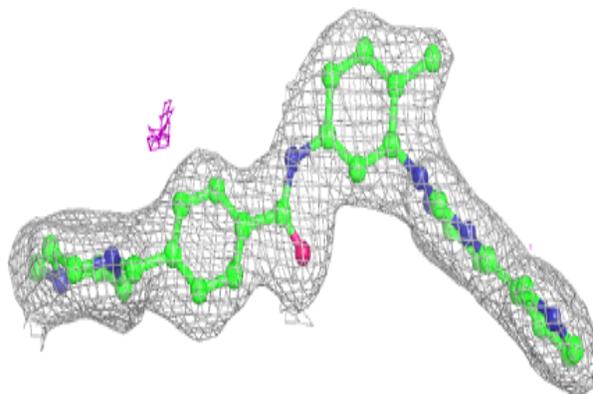


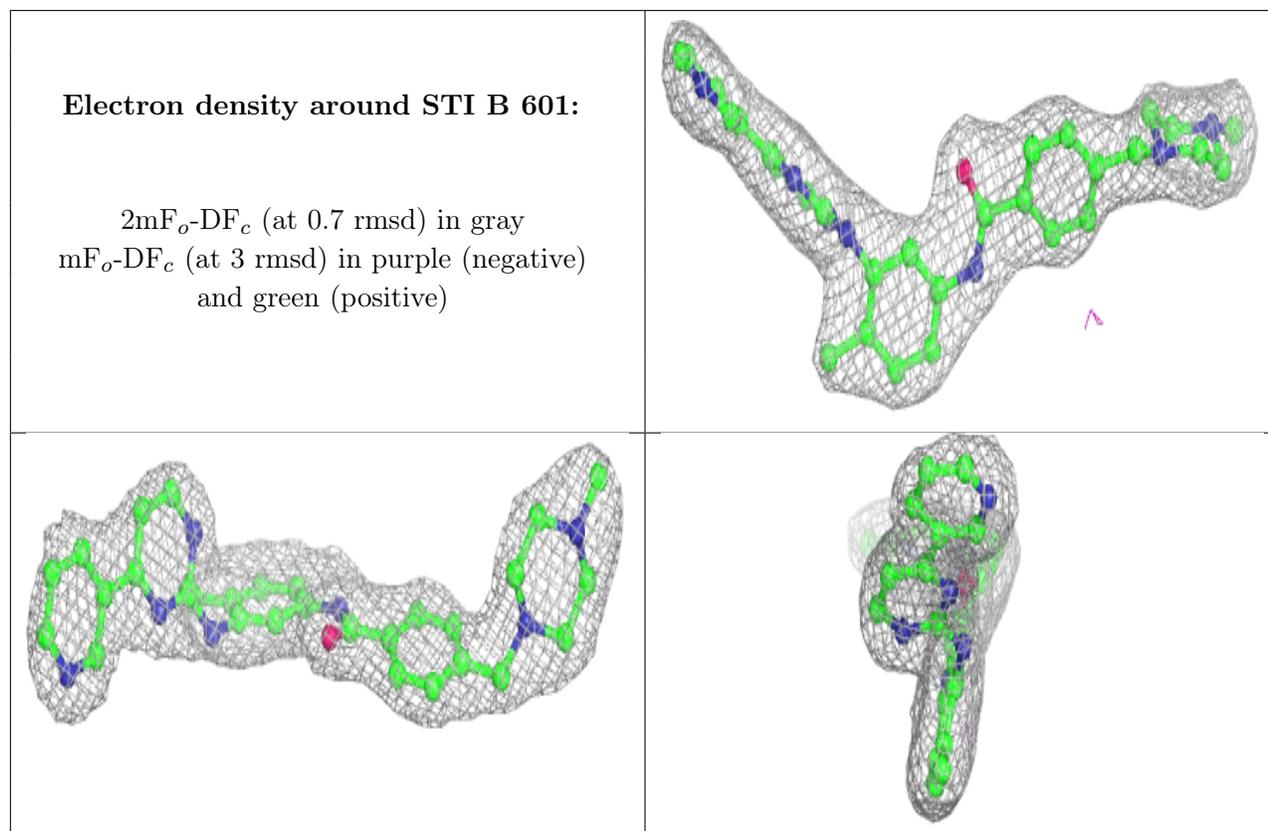
**Electron density around FYH A 602 (B):**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around STI A 603:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 5.5 Other polymers [i](#)

There are no such residues in this entry.